Micromagnetic simulations of hot-deformed Nd-Fe-B magnets after grain boundary diffusion process

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Nd-Fe-B permanent magnets based on $Nd_2Fe_{14}B$ phase (2:14:1) exhibit the largest maximum energy product among all types of permanent magnets and are widely used in energy conversion applications. The current problem of Nd-Fe-B magnets is their low room temperature coercivity and poor thermal stability that hinders their application at the elevated temperatures. One approach to enhance the coercivity is the infiltration of low melting point eutectic alloys into the grain boundaries of hot-deformed Nd-Fe-B magnets, known as eutectic grain boundary diffusion process (GBDP) [1]. However, the enhancement of coercivity has always been at the expense of a reduction in remanence. The question is, what are the desirable microstructural features to minimize the remanence deterioration while maintaining a maximum coercivity in hot-deformed Nd-Fe-B magnets? To answer this question, micromagnetic simulations can be used.

In this work, we developed a tomography-based micromagnetic model of hot-deformed Nd-Fe-B magnets which takes into account all real microstructural features of the magnets, *e.g.*, the intergranular phase (IGP) is subdivided into a ferromagnetic phase at the interfaces between 2:14:1 grains (indicated with blue color in Fig. 1a) and a non-magnetic phase located in the thick triple junctions (grey color). It allowed to reproduce realistic thickness and volume fraction of non-magnetic IGP forming after the GBDP as demonstrated in Figure 1a. Such an approach naturally considers the suppression of exchange coupling between grains and the deterioration of total magnetization. Our micromagnetic simulations suggest that full magnetic isolation of 2:14:1 grains is not necessarily beneficial to enhance coercivity while maintaining large remanence. As shown in Fig. 1b, more than 50 % coverage of 2:14:1 grains by non-magnetic IGP is sufficient to obtain high coercivity as long as thin IGPs are weakly ferromagnetic (blue curve). This results in a large coercivity of 3.0 T with a remanence of 1.3 T. However, in the case of grain boundaries with high magnetization, the coercivity is much lower and remains almost the same regardless the percentage of grain coverage by non-magnetic IGP (brown curve). Thus, GBDP is the most beneficial when it is accompanied by a suppression of the intergranular phase magnetism (*e.g.*, by adding Ga) otherwise is can lead to the deterioration of remanence mostly. In our report, these findings will be presented in more details giving a guideline for the efficient implementation of GBDP for hot-deformed magnets.

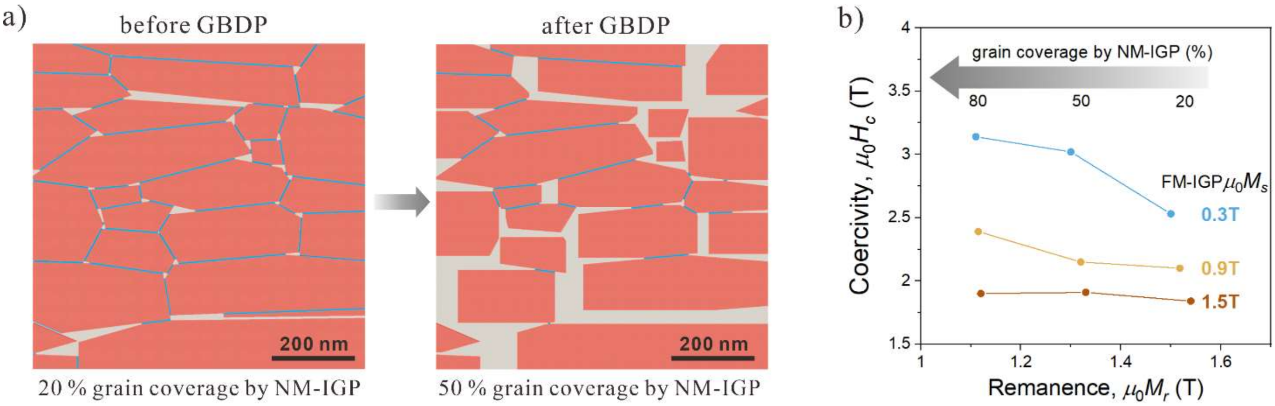

Figure 1: (a) Side-view image of tomography-based model of hot-deformed Nd-Fe-B magnets before and after imitation of grain boundary diffusion process (GBDP). Ferromagnetic intergranular phase (FM-IGP) is indicated in blue color, while non-magnetic intergranular phase (NM-IGP) is shown in grey color. (b) Comparison between coercivity and remanence for different values of FM-IGP magnetization with the increase of 2:14:1 grain coverage by NM-IGP.

References

[1] H. Sepehri-Amin, *et al*: High-coercivity ultrafine-grained anisotropic Nd–Fe–B magnets processed by hot deformation and the Nd–Cu grain boundary diffusion process. Acta Mater., 61, 6622–6634 (2013).